Reflections on the definition of the term 'substance' in the European Law on Substances

Helpdesk Focus: REACH

An unambiguous substance definition is a prerequisite for deciding on appropriate regulatory options for a substance. In the REACH, CLP and Biocides Regulation, substances are defined by their manufacture, i.e. as 'real substances'. This definition includes all constituents of a substance that is in principle not manufactured as an 'ideal substance' with a purity of 100 %. It has been shown that the real substance term alone is not sufficient to comprehensively regulate substances. In the following, the use of the two terms and the consequences in various areas of law will be examined in more detail.

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1 Introduction

For more than 50 years, chemical substances have been classified, labelled, evaluated in the European Union as well as worldwide and risk management measures have been taken for these substances respectively. It was and is important that chemical substances are subject to a unique substance definition, because only substances that are clearly defined can be identified as such, evaluated and regulated according to their risks. Under the EU REACH and CLP regulations, substances are defined according to the definition in Article 3 No. 1 REACH as chemical elements and compounds as they are manufactured, i.e. with impurities and possible stabilisers[1]. This substance definition is also increasingly used in related regulations. For example, the Biocides, PIC and POPs Regulations refer to this definition. The European Plant Protection Products Regulation uses a different but similar definition.

The central element of this definition is that substances are covered as they are manufactured. If, for the sake of simplicity, one initially disregards the possible stabilisers, a manufactured substance basically consists of a number of constituents, which are referred to as main constituents and impurities. In the rarest of cases, substances are manufactured with 100 % purity.

[1] substance: means a chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the stability of the substance or changing its composition.

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However, substances - as a result from manufacture - are also subject to legal regulations: They are subjected to an authorisation procedure, they are restricted, classified and labelled or approved. Accordingly, they are included in lists and named in annexes. However, these substances are not listed as they actually occur - i.e. with all main constituents and impurities they contain. Instead, they are identified according to more general criteria. As a rule, this is done by naming one or more main constituents (in the case of the so-called mono- or multi-constituent substances). Or, they are identified by their manufacturing process (especially relevant for so-called UVCBs[2] - however, these are not the subject of these reflections).

This shows that a uniform substance definition cannot cover all areas of substance regulation without distinction. Therefore, in official practice, the concept of ideal and real substances has been developed, which will be explained below. Real substances are those that actually occur during manufacture or are actually extracted. As a rule, these consist of several or many ideal substances.

Under REACH, real substances are registered; the ideal substances contained are to be identified in the registration dossier. Risk management measures (as in the lists of substances in Annexes XIV and XVII of the REACH Regulation or in Annex VI of the CLP Regulation) are usually provided for ideal substances. These measures then apply to all real substances containing these ideal substances above a certain concentration.

Although the definition of a substance is unambiguous and only covers the manufactured substance with its impurities, the term is used in different contexts with different meanings. The key question however is always whether the real substance is addressed or whether it is not rather the eponymous part, the main constituent, that is at the centre of the consideration, i.e. the ideal substance. A possible solution to this problem is presented in the following, whereby the central element consists in a specification of the substance definition, which distinguishes between ideal and real substances. **Only those substances are considered whose qualitative and quantitative composition is known: defined substances with one main constituent.**

2 Real and ideal substance

Due to the different use of the term "substance" in European substance law, the following clarification of the term "substance" is proposed:

1. the substance as it is manufactured = **real substance** (in the sense of the substance definition in Article 3 No. 1 REACH)
2. substance, in the sense of constituent = **ideal substance**

The ideal substance is considered to be the 100% pure substance that can be uniquely identified by a molecular formula and an IUPAC name. The ideal substance level is the level at which a unique IUPAC name is assigned to a molecular structure or a unique CAS No. is assigned by the Chemical Abstract Service. At this point, this number in itself has no legal relevance, it only identifies a chemical structure, the ideal substance. Manufactured ideal substances practically do not occur in reality. They are merely an instrument for regulating chemicals.

Nevertheless, the CAS No., i.e. an ideal substance identifier, is also adopted for **real substances** under REACH by laying down rules. For this purpose, the conditions were determined

[2] UVCB: Unknown or Variable composition, Complex reaction products or Biological materials

(80 % rule[3]) under which an ideal substance is considered to be the main constituent and in this function determines the identity of the real substance. The rules for determining the identity of substances have been agreed between ECHA and the Member States in the Guidance on identification and naming of substances under REACH and CLP.

The following examples illustrate how the substance definition has been applied differently in the various processes (registration, authorisation, restriction) of the **REACH Regulation**, without addressing the distinction between ideal substances and real substances. Furthermore, it is shown how the substance definition should be correctly applied with these extensions:

- **EINECS** (European INventory of Existing Commercial chemical Substances) forms the basis for the definition of phase-in substances in Article 3(20). EINECS lists the substances commercially available on the European market between 1 January 1971 and 18 September 1981, defined by a CAS No., a CAS Name and an EC No.. Behind such an entry there is in about 80% of the cases a certain defined chemical structure, i.e. a 100% pure substance. This entry is used by convention for the identification of the named commercially available substances with more or less impurities.

  The **EINECS** list is therefore, although the substances are listed without information on purity and impurities, defacto a **real substance list**. A prerequisite for the use of the list is that a regulation exists that establishes the relationship between ideal substances and real substances. This rule is the 80% rule for defined substances.

- Article 3(15) defines **intermediates**
  intermediate: means a substance that is manufactured for and consumed in or used for chemical processing in order to be transformed into another substance.

  This means that the substance is chemically converted in order to be categorized as an intermediate. In practice, however, only the main constituent of the **real substance** is considered, which means that if it is chemically converted, the definition is considered to be fulfilled. The legal text would have to read correctly, taking into account the extended concept of substance:

  intermediate: means a substance that is manufactured for chemical processing and **the main constituent** of which is consumed in or used for chemical processing in order to be transformed into another substance.

- **Article 6** sets out the conditions under which a manufactured or imported substance (**real substance**) must be registered. Through the link to manufacture, the substance is considered in its entirety with impurities and necessary additives.

- **Article 7(1)** establishes the obligation to register substances (real substances) intended to be released from articles under normal or reasonably foreseeable conditions of use. The trigger for the obligation, however, is the ideal substance, the eponymous main constituent.

[3] The 80% rule states that a defined real substance that contains a main constituent (ideal substance) of at least 80% is identified and named via it.
See „Guidance for identification and naming of substances under REACH and CLP“ *https://echa.europa.eu/en/guidance-documents/guidance-on-reach*

- **Article 33** regulates the duty to disclose information:
  Any supplier of an article containing a substance meeting the criteria in Article 57 and identified in accordance with Article 59(1) in a concentration above 0,1% weight by weight (w/w) shall provide the recipient of the article with sufficient information, available to the supplier, to allow safe use of the article including, as a minimum, the name of that substance.
  The candidate list contains substances of very high concern (SVHC). They are identified here by their CAS No. and the CAS or IUPAC name. As a rule, no information on purity and impurities is given.
  The **candidate list** is therefore an **ideal substances list**[4]. However, due to the application of the 80% rule, this list applies first and foremost to real substances. This means that a manufacturer of a real substance identified via a CAS No. must observe the legal obligations when using this real substance.
  Ultimately, however, in the case of information obligations according to Article 33, the information on the ideal substance is always passed on, mostly in the form of the CAS No. This is because, as in the case of mixtures (see below), the original relation of main constituents and impurities of a real substance is also not maintained in articles, or in the article, the concrete constituents of the individual real substances are not (any longer) known and assignable and/or irrelevant for the management measure. Therefore, if an analysis is necessary to determine the SVHC content in an article, only the ideal substance is "searched" for.

- **Annex XIV** is the list of substances for whose use an authorisation must have been granted. The substances on this list are identified by their CAS No. and CAS or IUPAC name. As a rule, no information on purity and impurities is given, i.e. Annex XIV should be a **list of ideal substances**. However, this concept was not consistently applied, as can be seen from individual entries[5]. **Authorisation obligations** are triggered when a **real substance** is used (in reality, only real substances are used), which is usually identified by an ideal substance in Annex XIV.
  This further means that a real substance that "only" contains an Annex XIV substance as an impurity does not lead to an authorisation requirement for the use of this real substance, even if it poses an identical risk as the use of a mixture containing this substance as a real substance (see below).

- **Annex XVII** contains substances or groups of substances subject to restriction. The substances are identified by their CAS No. and CAS or IUPAC name. As a rule, no information on purity and impurities is given. This means that Annex XVII is a list of ideal substances. This Annex contains entries restricting substances as such or as constituents in other substances, e.g. entry 28:
  Substances which are classified as carcinogen category 1A or 1B in Part 3 of Annex VI to Regulation (EC) No 1272/2008 and are listed in Appendix 1 or Appendix 2, respectively
  1. *Shall not be placed on the market, or used,*
  - *as substances,*
  - *as constituents of other substances, or,*
  - *in mixtures, ...*

  Here it becomes clear that Annex XVII explicitly applies the extended substance definition to a number of restrictions. This means that in the example, both real substances as manufactured and real substances containing a CMR ideal substance of category 1 as a constituent in the form of an impurity (in contrast to the authorisation requirement) are addressed.

[4] However, entries for multi-component substances and UVCB substances are also sometimes found.
[5] Entry 42 in Annex XIV: 4-(1,1,3,3-tetramethylbutyl)phenol, ethoxylated [covers well-defined substances, UVCB substances, polymers and homologues].

Furthermore, mixtures containing a CMR substance are covered by this entry. This can be both, the real substance and an impurity of the real substance used for the formulation. This was already common regulatory practice before REACH and the introduction of the substance definition under the predecessor regulation, Directive 76/769/EEC.

The CLP Regulation, which has taken over the substance definition from REACH, also uses the substance definition differently:

- Annex VI, the List of Harmonised Classifications and Labelling of Dangerous Substances, is an ideal substance list in which substances are identified by CAS No., EC No. and chemical name.
  In Annex VI CLP the classification and labelling of the ideal substance is given without specification of purity and impurities. This ideal substance is used as the main constituent of a substance for the classification of the real substance (assumption here: the impurities have no hazardous properties).

- In paragraph 1 of Article 11, the following wording is used: "Where a substance contains another substance, itself classified as hazardous, whether in the form of an identified impurity, ..."
  This means that the substance definition is used here in the extended meaning, as a real substance cannot contain another manufactured substance. After applying the extended concept of substance, the above formulation would have to read
  "If a real substance contains an ideal substance, classified as hazardous in itself, in the form of an identified impurity ...".
  In addition, paragraph 2 of Article 11 classifies a mixture on the basis of a substance classified as hazardous if it is present either as a constituent or in the form of an identified impurity or additive. This sentence should read: "If a mixture contains a real substance classified on the basis of either an ideal substance (main constituent or identified impurity) or an additive ...".

- Article 38 says something about the necessary information required in the context of opinions and decisions "referred to in Article 37(4) and any decision according to Article 37(5)": inter alia "any other parameter enabling an assessment to be made of the health or environmental hazard of mixtures containing the hazardous substance in question or of substances containing such hazardous substances as identified impurities, additives and constituents".
  This sentence would have to be formulated as follows for an unambiguous statement: „any other parameter enabling an assessment to be made of the health or environmental hazard of mixtures containing the hazardous real substance in question or of real substances containing such hazardous constituents (ideal substances) as identified impurities, additives and constituents“

- Corresponding ideal substance lists can also be found in other legal acts of European substance law, such as the PIC Regulation or the POP Regulation. These lists are usually ideal substances list.

This non-exhaustive list of examples clarifies that the substance definition as determined in REACH or CLP, without the proposed detailing, is not in itself suitable to clearly describe the cases outlined. It is obvious that both substances in the sense of the definition, i.e. as manufactured with impurities, and substances in the sense of constituents are to be regulated under REACH and CLP.

The term mixture itself in the sense of Article 3 No. 2 REACH does not need to be further specified, it includes the formulation of real substances. In practice, it must be taken into account that the original allocation of the constituents of a real substance in the mixture is lost. This means that the real substances within a mixture can no longer be detected analytically. All that remains is to trace the manufacturing process in order to carry out this allocation.

This is summarised once again in the following figure 1:

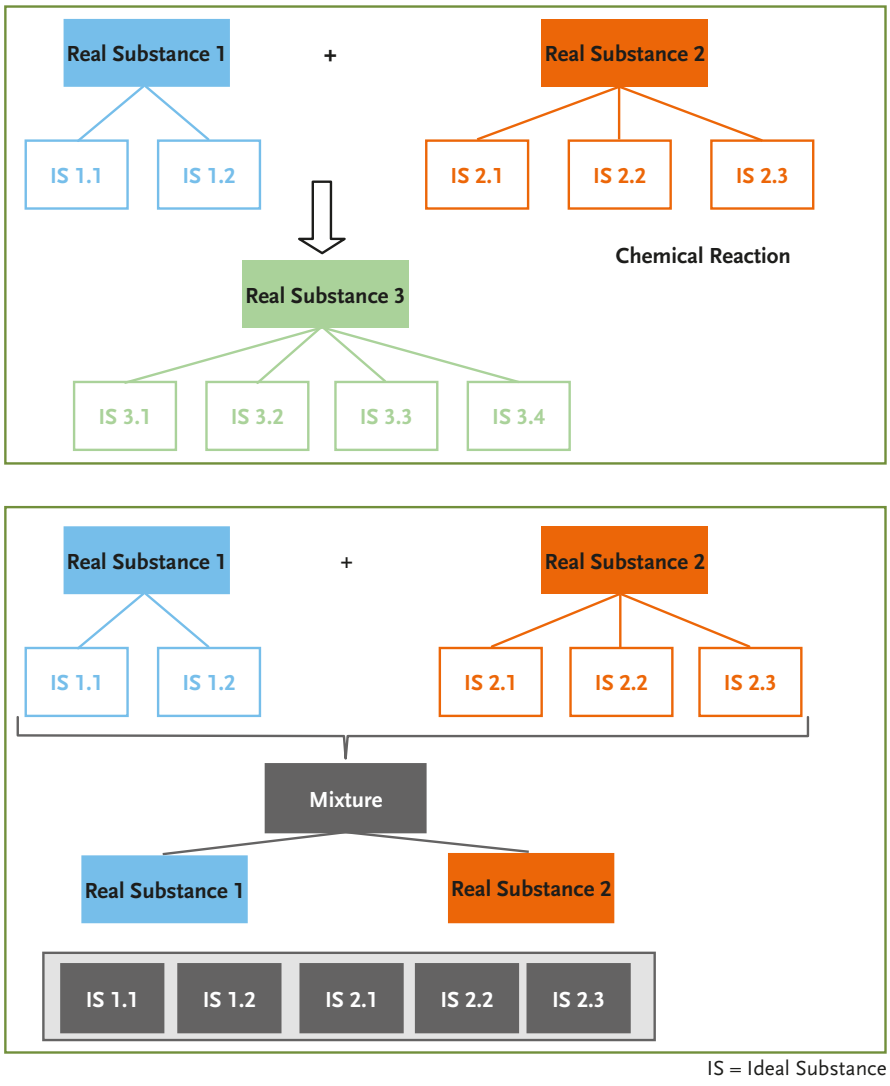

Fig. 1 Difference between the mixture and substance definition

This differentiated consideration of the substance definition into ideal and real substances, which was derived here for defined substances with one main constituent, ultimately also allows for substances with several constituents up to complex substances to be regulated.

3 Regulation of substances and mixtures

From the point of view of the risk posed by a substance or a mixture, it is irrelevant whether a formulated mixture or a real substance identical in its composition up to the ideal substance level is present (see Figure 2).

If one analyses both materials in Fig. 2 "real substance" and "mixture", regardless of the knowledge about their manufacture or formulation, one would conclude in both cases that

they are identical materials in view to their composition. As described above, in the case of a mixture, the relation between the ideal and real substances of the starting materials is lost if one has no knowledge of how the mixture was formulated. **The potential hazard posed by both materials is identical**.

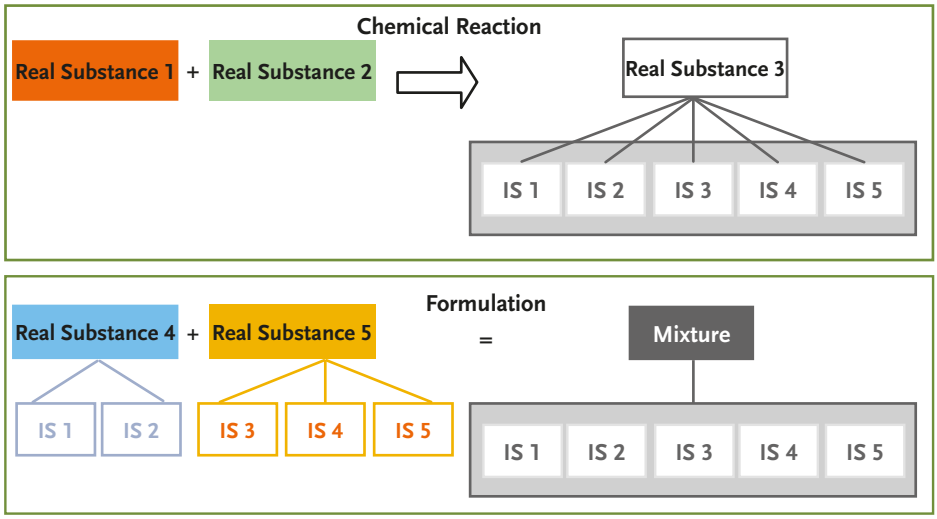

Fig. 2 Regulation - Comparison substance/mixture

IS = Ideal Substance

In practice, substances are tested more often than mixtures, and the latter are then classified on the basis of the constituents/components they contain. This means that complex, identically composed substances and mixtures with a high number of constituents/components may have different classifications. The tested complex substance may show no effect under the test conditions, whereas the mixture has to be classified according to the CLP Regulation on the basis of the constituents/components it contains.
However, it should be noted that according to the CLP Regulation, even in the case of testing of a substance (or mixture), the properties of the **constituents/components** of the material have to be considered for classification and labelling purposes.

4 Conclusion

The explanations show that the substance definition in European substance law has partly grown historically and is not uniformly used. At least, the term substance cannot be used in different contexts without an interpretation of whether it is an ideal or real substance.

Figure 3 shows examples of cases and regulatory procedures in which substances have a different substance meaning in the sense of ideal and real substance.

When applying the substance definition, it must therefore always be verified whether the real or the ideal substance is meant. The ideal substance is often referred to as "constituent" in the legal text.

It would be desirable if the substance definition was adapted and uniformly implemented in a future adaptation of the legal text. The REACH Regulation, as the basic text of substance law, is of particular importance. Here, the basic terms and definitions should already be laid down in the definition section and then consistently adapted. It could then be expected that these would subsequently be adopted in the other legal regulations.

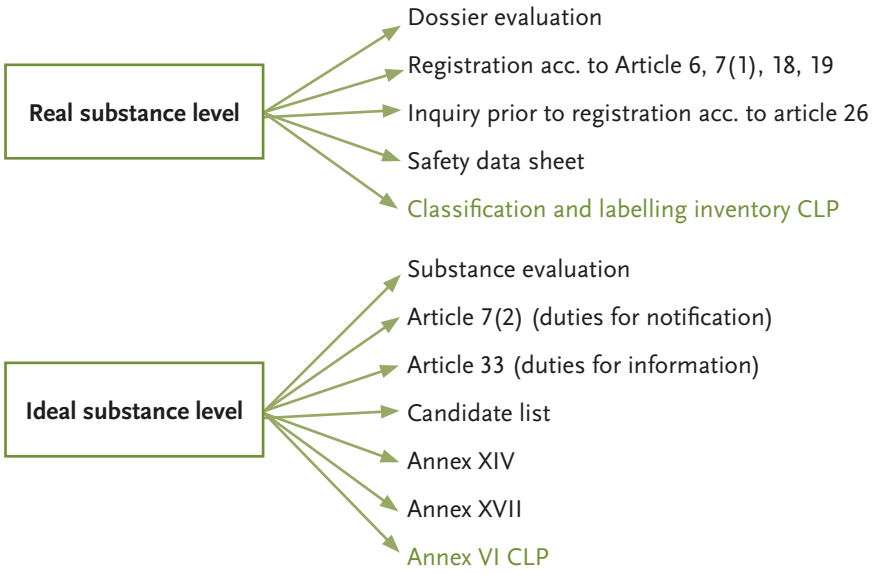

Fig. 3 Substance definition in processes under REACH and CLP

A clear understanding of the substance definition, but above all a uniform understanding, will be decisive for successfully implementing the concept of "one substance, one assessment" contained in the European Commission's new chemicals strategy for a pollution-free environment. As challenging as this will be in any case, it presupposes right from the start that the basis of what is being assessed is consistent.

The report reflects the views of the authors. The responsibility for the content of this publication lies with the authors.

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